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Who we are

The University of Illinois at Urbana-Champaign's National Center for Supercomputing Applications (NCSA), one of the five original centers in the National Science Foundation's Supercomputer Centers Program, opened its doors in January 1986. Over the years NCSA has contributed significantly to the birth and growth of the worldwide cyberinfrastructure for science and engineering, operating some of the world's most powerful supercomputers and developing the software infrastructure needed to efficiently use them.

That tradition continues as the center, Illinois, IBM, and their partners in the Great Lakes Consortium for Petascale Computation develop what is expected to be the first computer dedicated to open scientific research capable of sustaining more than one petaflop, or one quadrillion calculations per second. Called Blue Waters, the system will come online in 2011. It will be dedicated to massive simulations and data analysis projects that will improve our society, health, environment, and economic competitiveness. NCSA and the consortium will also work with research communities to create the new software technologies, scientific applications, and educational programs needed to take full advantage of this new system.

Blue Waters will benefit from NCSA's ongoing focus on cyberenvironments, cyber-resources, and innovative systems research. Cyberenvironments give research communities the means to fully exploit the extraordinary resources available on the internet (computing systems, data sources and stores, and tools). Cyber-resources ensure computing, data, and networking resources are available to solve the most demanding science and engineering problems and that the solutions are obtained in a timely manner. Innovative systems research involves testing and evaluating the performance of emerging computing systems for scientific and engineering applications.

NCSA also leads efforts to develop a secure national cyberinfrastructure. Through the National Center for Advanced Secure Systems Research, a project funded by the Office of Naval Research, critical cybersecurity and infrastructure needs and research requirements are addressed. In addition, NCSA is a key partner in the National Science Foundation's TeraGrid project, a $150 million effort to offer researchers remote access to some of the fastest unclassified supercomputers as well as an unparalleled array of visualization tools, application software, sensors and instruments, and mass storage devices.

The center also leaves its mark through the development of networking, visualization, storage, data management, data mining, and collaboration software. The prime example of this influence is NCSA Mosaic, which was the first graphical Web browser widely available to the general public. NCSA visualizations, meanwhile, have been a part of productions by the likes of PBS's NOVA and the Discovery Channel. Through its Private Sector Program, top researchers explore the newest hardware and software, virtual prototyping, visualization, networking, and data mining to help U.S. industries maintain a competitive edge in the global economy.

Support for NCSA is provided by the National Science Foundation, the state of Illinois, industrial partners, and other federal agencies. For more information, see www.ncsa.illinois.edu.

On the cover

Professor Arif Masud and his team in the civil and environmental engineering department at the University of Illinois at Urbana-Champaign are developing mathematically robust and computationally economic fluid-structure interaction techniques with the assistance of NCSA, so researchers can economically obtain accurate solutions. One of their projects used NCSA's Cobalt to test algorithms modeling aircraft pressure, velocity, and vorticity around YF-17 aircraft. The center's Advanced Applications Support visualization group helped to visualize the results. Learn more by turning to page 28.

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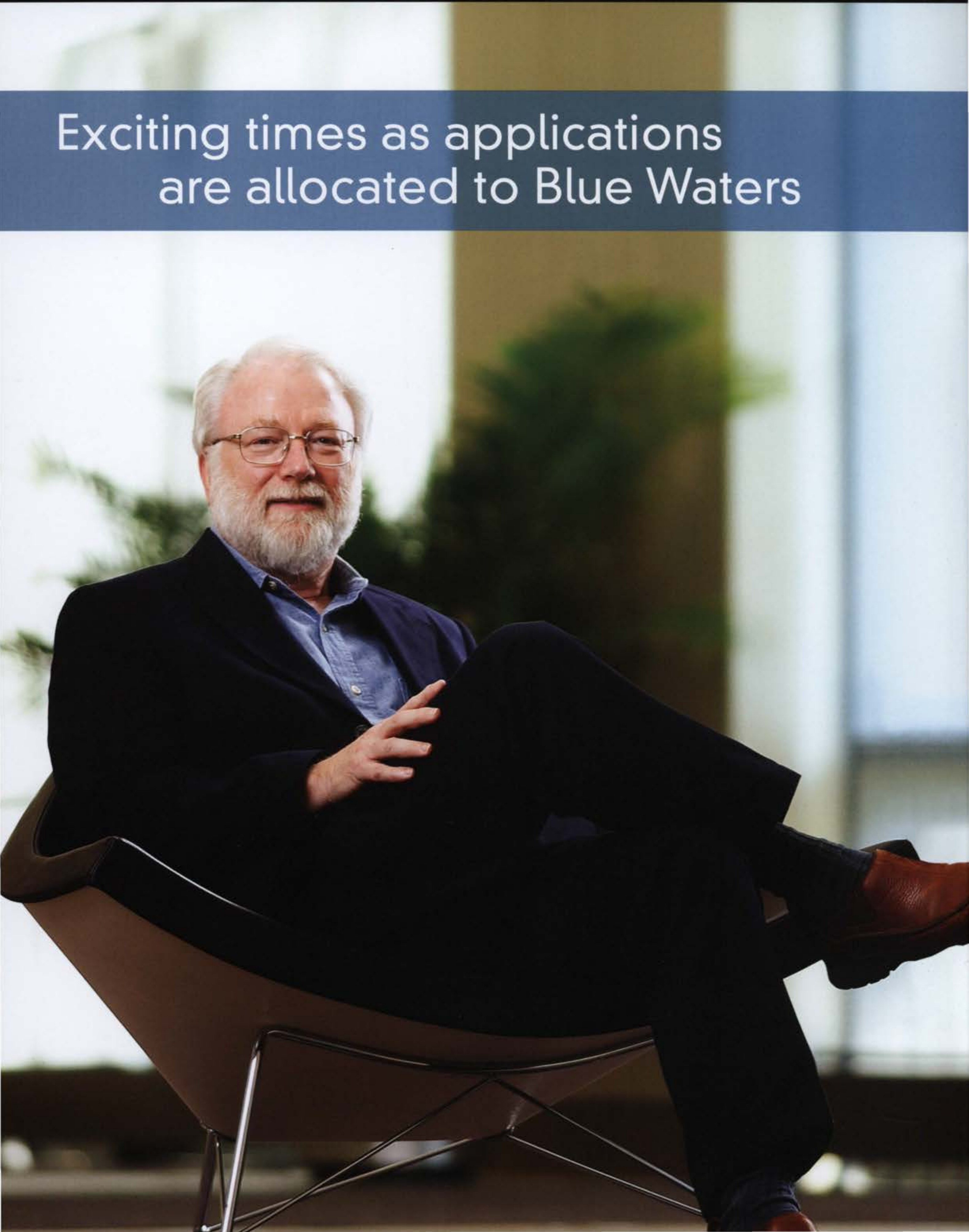
Exciting times as applications are allocated to Blue Waters



An Expert Opinion

"Early engagement with the PRAC awardees will ensure that the research community can take full advantage of the extraordinary capabilities of Blue Waters to solve the most challenging and critical problems in science and engineering."

EARLIER THIS SUMMER, excitement started to build for the Blue Waters sustained petascale computing system as the National Science Foundation announced the first science teams to receive preliminary Petascale Computing Resource Allocations (PRACs) for Blue Waters. Each PRAC award identifies a scientific challenge requiring advanced modeling and simulation capabilities that can only be provided by a system with a sustained performance approaching a petaflop. There is a listing of the initial awards in this issue, with more awards to follow over the next two years.

With the PRAC announcements—along with the progress in the Blue Waters system design and implementation—Blue Waters project staff will be engaging with scientists and engineers regarding specific applications targeted for Blue Waters. The project team has developed a comprehensive, four-phase approach to support the PRACs before, during, and after deployment. NCSA has a team of application and user support staffs ready to assist the PRAC science teams with porting and tuning, even re-engineering, their applications to make full use of the novel hardware and software available on Blue Waters. The process begins with performance modeling and processor and network simulation to explore the benefits of different approaches, then moves on to the insights enabled by early hardware experiments, and eventually final optimization and tuning on the Blue Waters system itself. The Blue Waters project is collaborating with two performance modeling groups, Los Alamos National Laboratory's Performance and Architecture Laboratory (PAL) and UC San Diego's Performance Modeling and Characterization (PMaC) group, who are both able to work with selected PRAC codes to understand and optimize the performance of the applications.

At the same time, PRAC scientists will be able to use a Blue Waters interim system, a 2,000-core IBM Power 5+ system called BluePrint. While this system does not approach the computational or storage power of Blue Waters, it will have an environment similar in many ways to what Blue Waters will be providing, so PRAC scientists can acclimate themselves to the programming environment. BluePrint will also be running early releases of some expanded Blue Waters computing system software between now and the deployment of Blue Waters. Periodically, Blue Waters staff will be holding training workshops on topics such as the Mambo (processor) and BigSim simulation environments, performance monitoring and analysis tools, I/O strategies, and library routines.

A Blue Waters Interim System, a 2,000-core IBM Power 5+ system called BluePrint, installed at NCSA.

During the next year, the Blue Waters team, through a series of meetings, workshops, and other interactions, will work to understand the specific goals and needs of each PRAC team, and will use this information to help optimize the Blue Waters configuration and services. This information will guide the Blue Waters project as it makes Blue Waters one of the world's most powerful and effective tools for computational science.

The Blue Waters team envisions a seamless transition for the PRAC teams from the development phase of Blue Waters to the multi-year production phase of the system. The same high-quality service that users of other NCSA systems have come to know will be available to all of the scientists and engineers using Blue Waters.

Today, Blue Waters is more than halfway through its development and deployment phase. Early engagement with the PRAC awardees will ensure that the research community can take full advantage of the extraordinary capabilities of Blue Waters to solve the most challenging and critical problems in science and engineering. Stay tuned! ◻

Thom Dunning
Director, NCSA

Questions & Answers

Power to change everyday life

Modeling and simulation are an integral part of modern research and development. Tom Lange, director of corporate research and development modeling and simulation at NCSA's newest Private Sector Program (PSP) partner, Procter & Gamble, presented at the PSP partners meeting in May. He shares with *Access*' Barbara Jewett some key points from that presentation as well as other thoughts on how high-performance computing impacts not just his work with one of the world's largest corporations, but also U.S. innovation and competitiveness.

Q: You were part of a Council on Competitiveness working group that examined high-performance computing (HPC) and U.S. industry. Why is HPC important to industry in general, and to Procter & Gamble in particular?

A: The Council on Competitiveness is a nonpartisan, nongovernmental group of corporate CEOs, university presidents, and labor leaders working to ensure U.S. prosperity. Why is HPC important to the council and to P&G? It really comes back to this innovation cycle: design, build, fly, crash, fix. People usually understand this for an automobile or an airplane, but it is really hard for most people to wrap their minds around this for disposable diapers or laundry detergent. Consumer products manufacturers have the same motivation to do modeling and simulation as most durable goods manufacturers.

If you are stuck in a physical "only" learning cycle, development costs too much and takes too long. It takes time to build prototypes, which are a one-time use, and you need a huge testing infrastructure. Sometimes that limits innovation because you can't bet it all on the next idea; you have to be a little more disciplined than that for your shareholders.

Q: What could P&G and other companies do if you had unlimited advanced computing resources in the modeling and simulation area?

A: What if we could predict, from *ab initio* quantum methods, chemical erosion kinetics? Why would P&G care about that? Hairspray in metal cans is expensive. I'd like to put it in a less expensive bottle, but I can't put it there for chemical corrosion reasons.

What if we could do with less wrapping, less cardboard, less plastic, and less metal in our packaging? I'll bet up to 20 percent of the packaging in our grocery stores is insurance. The truth is, it's there because we haven't done the engineering to take it out.

What about car crashes? I'm glad safety experts do the crash tests with the dummy. But what if we could predict hematoma and stop predicting just the G-forces to a dummy's head. Can we predict hematoma? That requires more computing. You don't need just models of the head, you also have to have models of the brain, and a fluid structure interaction where you account for that.

We could solve the biggest, the most complex problems with more computing power. And maybe someone could finally create a plastic fork where that bottom tine doesn't break off!

Q: Why aren't we doing some of those things now? We have the compute power to tackle many of these problems.

A: Lack of application software. That's the issue from my chair. Software for parallel processing is our problem. For example, we don't have the software to simultaneously do spatial and temporal decomposition so I can affordably track molecules and machinery at the same time. There is also an affordability issue related to business models.

Education is also an opportunity. We don't have engineering and science graduates that are computationally aware at the bachelor's and master's levels. The Ph.D. level is fine. But at the lower levels they are being taught, I regret to say, very similarly to the way I was taught a long time ago—and I took my first college chemistry test with a slide rule.

Why is this happening? Because the universities don't have the software either. You know, there are a lot of "why's." Like why are colleges and universities still emphasizing teaching serial programming in computer science classes when parallel is the way the world is going?

Q: So what are you doing with modeling and simulation at P&G?

A: When consumers get products home, the products need to perform as expected or as advertised. Performance in my world often means leveraging fundamental science and engineering contradictions.

I need Charmin to be soft but strong. Diapers that breathe yet contain. Moisturizing lotions that stay put when applied but are easy to squeeze. Who wants toothpaste that falls off the brush before reaching the mouth?

With HPC, modeling and simulation lets us more quickly create these products, transforming everyday life. I can replace slow and expensive learning cycles with faster and cheaper virtual realism. We don't yet do everything virtually, but I'm trying.

I have computing machines that are about a decade behind leadership-class machines. I don't apologize for this. P&G is not going to be on the leading edge like government labs or NSF machines like Blue Waters. But through collaborations with government labs and with centers like NCSA, we can access leadership-class compute power for problems like very large molecular dynamics simulations (oil-water surfactant mixtures), for large computational fluid dynamics problems with flow-through porous media, or finite element analysis for very complex machines with hundreds of thousands of moving parts.

Q: How do you justify the return on investment in HPC within an industrial setting?

A: Every year our department does a business impact study that is reviewed with our finance department. This study is shown to our senior leadership. It includes things like capital avoidance and innovation cost savings. It includes the business impact of new products or businesses that modeling helped make possible. We might not have been the only contributor but we were a necessary contributor.

Q: Can you give a specific example where P&G benefitted from HPC in R&D?

A: We used HPC, primarily finite element analysis, when we transitioned Folgers coffee from metal cans to plastic containers a few years ago. Consumers think it's great we made a container with handles and flat panels, giving it a cool look. The truth is the flat panels on the front were put there to solve a stress problem.

After we seal the can at the factory, the coffee continues to give off gas, which builds up and exerts pressure against the container. A metal can is able to handle that pressure, but not an affordable plastic one.

Why not leave it in a metal can? Oil from the coffee in the presence of oxygen makes it go stale in metal. So a one-way check valve in the plastic container that swings open to relieve the internal pressure but doesn't let oxygen back in the container solved the problem. However, the check valve gives you another problem during shipping.

When the truck goes up over the mountains, the pressure drops, gas builds in the container and is released by the valve. Going down, the outside pressure rises again, greatly exceeding the now lower pressure within the canister. Because the air can't get back in to equalize the inside and outside pressure, the canister implodes, basically crushing itself.

Stores don't want to put crushed containers on their shelves, and consumers certainly don't want to buy them. Using modeling and simulation, we helped engineer a solution: flat panels that fit on the side of the canister. When the canister starts to implode, these panels shrink as well and evenly distribute the stress. The bottom and top remain round, and the side panels flatten out a bit and look slightly square. Implosion problem solved.

Simulations showed there was still enough stress generated that an area around the canister lid would crack. As the crack spread, the whole lid collapsed and came off. You could potentially wind up with a disaster; imagine an entire truckload of coffee canisters with no tops. The traditional approach to solving this problem would be to assemble a team to discuss and devise designs, make numerous prototypes, fill them with coffee, load them in a truck, and ship them over the mountains to see what happens. That takes four to six months before you see your results. By using HPC to model various canister/lid designs and try them out in simulated environments, very shortly we had a canister and lid that performs as it should.

Q: But your modeling and simulation department is about more than just new product development and package designs, isn't it?

A: We use a variety of computational science and engineering codes for all sorts of problems.

We do computational chemistry to better understand our formulations. This was very important during Hurricane Katrina when our surfactant supply was threatened. We used models to reformulate very frequently and maintained our supply to our customers through that entire period. And maintained the cleaning performance of a pivotal brand. □

More information www.pg.com/science/index.shtml
www.compete.org

In the wind

By Barbara Jewett

Reducing wind turbine noise while maintaining performance is a wind industry challenge. Using NCSA's Mercury, a Georgia Tech team is contributing to the solution.

IT'S SO QUIET. That's my first thought as I stand on the road in the middle of a 240 turbine wind farm a few miles from my home, watching the blades slowly rotating in the breeze.

My family's been following the installation of the turbines. Today as we drive over to peek at the project's progress we see the giant blades are moving. We scramble from the van as soon as it stops, uncertain what to expect. As we stand in awe at the sight of hundreds of white blades slowing going round and round in the azure sky, the normal Sunday afternoon quiet of the rural road is broken only by the pinging of the van's cooling engine.

"Just because you didn't hear any sounds from the wind turbines doesn't mean they weren't generating noise," says Georgia Institute of Technology aerospace engineering associate professor Marilyn Smith. Her team is developing a tool they hope will advance wind turbine design and analysis, which includes measuring low-frequency noise—those sounds below the normal limit of human hearing.

The quiet noise

While modern versions may be quieter than their predecessors, reducing wind turbine noise while maintaining performance is still a challenge. In fact, some in the wind industry say it is the greatest challenge advocates face in gaining widespread wind turbine acceptance as the U.S. transitions from traditional carbon-based fuels such as coal and natural gas to more sustainable forms of energy like wind.

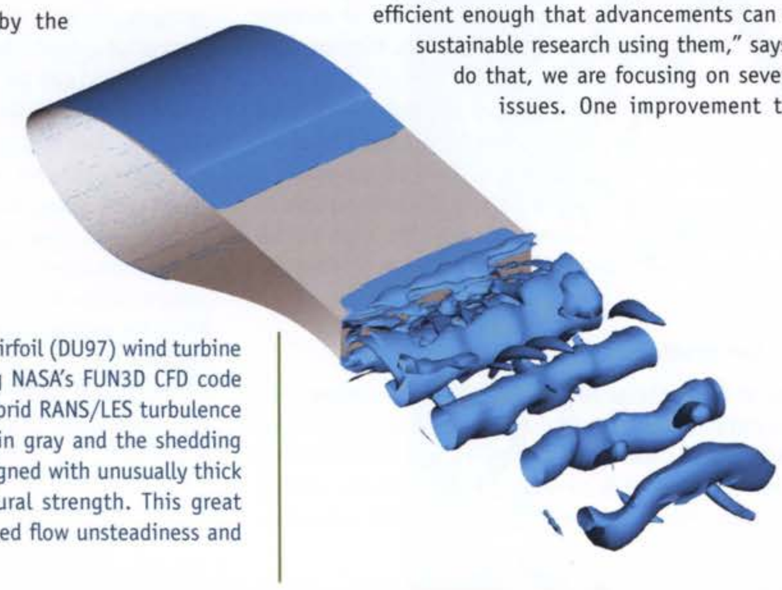
"There has been some speculation by the public that wind turbines—that is, the low frequency noise generated by their rotating blades—may be causing some health issues, such as migraines. When a wind turbine is exposed to wind, a pressure differential is created on the rotor blade, which drives the blade rotation, but is also a source of noise. An example that most people are familiar with is exiting or entering a building via revolving doors. You can feel the pressure change, and sometimes hear an accompanying noise as the pressure equalizes between the building and external atmosphere. The tools that we are developing can be used by other researchers who can use them to answer questions such as the physiological effects of wind turbine noise," says Smith.

Her team is using NCSA resources to develop methods for use in both design and analysis of wind turbines. Their tool will allow wind turbine manufacturers and researchers to examine not only turbine blades but also entire wind turbine structures and potentially wind farms.

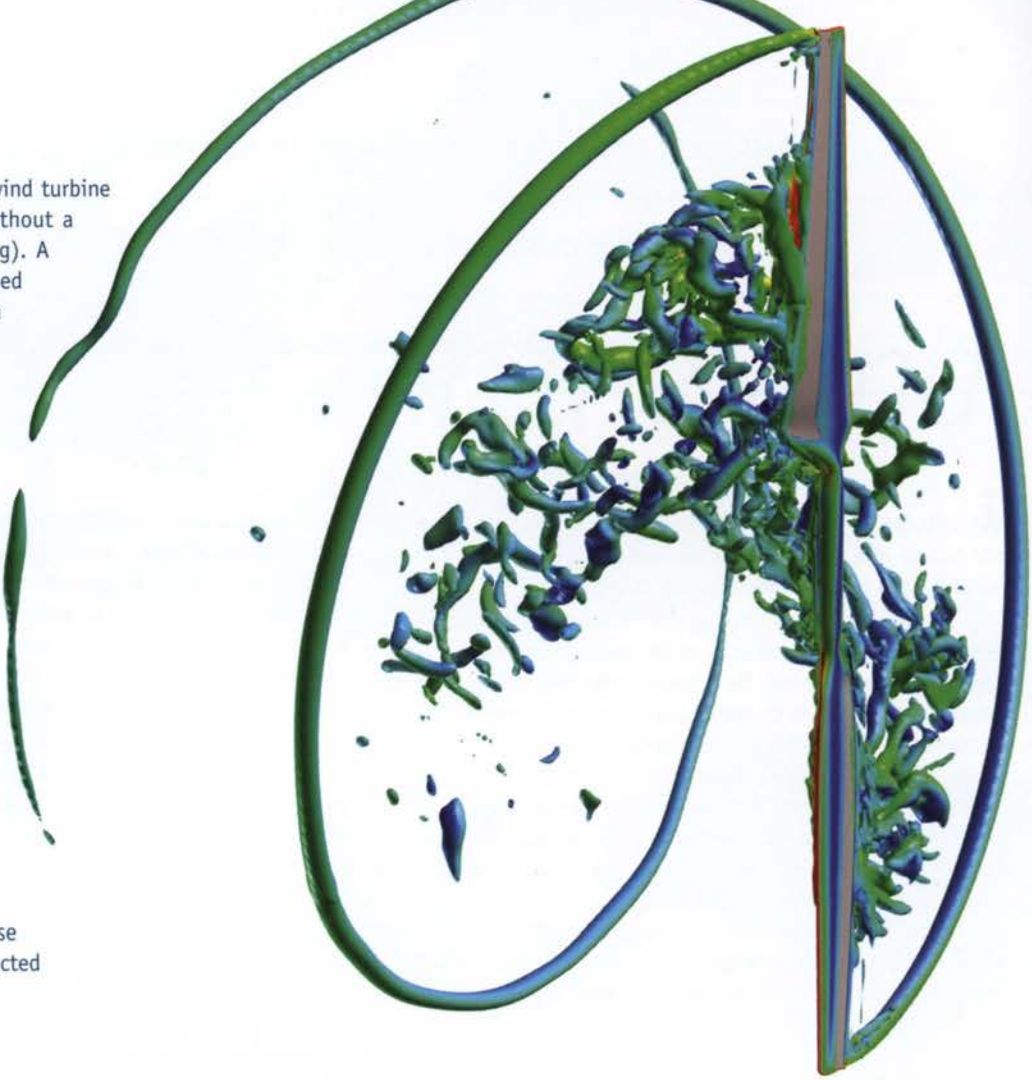
Aerodynamic factors

The primary source of noise is the aerodynamic effects—that pressure differential Smith spoke of—and is known as aeroacoustic noise. Various factors influence the strength of the aeroacoustic noise, including inflow turbulence, turbine blade elasticity, and tip speeds. The prediction of their relative effects is incredibly challenging and draws upon a multitude of engineering fields including aerodynamics, turbulence, structural dynamics, material science, and atmospheric science.

"Our focus is not so much on solving the world's problems but developing tools that have high enough fidelity yet are efficient enough that advancements can be made in sustainable research using them," says Smith. "To do that, we are focusing on several different issues. One improvement that we are



Simulation of an infinite-span "flatback" airfoil (DU97) wind turbine airfoil designed by Delft University using NASA's FUN3D CFD code modified by Georgia Tech to include a hybrid RANS/LES turbulence model. The airfoil geometry is is shown in gray and the shedding vortices in blue. Flatback airfoils are designed with unusually thick bases intended to increase their structural strength. This great stiffness comes at the expense of increased flow unsteadiness and possible increased noise.



Right: The modeling of a two-bladed wind turbine rotor using NASA's OVERFLOW code without a tower or nacelle (the gear box housing). A hybrid LES turbulence model was developed and implemented by the research team and employed here. This simulation is used to study the wake dynamics behind the rotating blades of a wind turbine. The blades can be seen in the forefront in gray; very distinct tip-vortices are seen emitting from their ends. Massive flow separation is evident inboard on the rotor.

Bottom Right: The interaction of the tower and nacelle with the rotating blades is simulated here in a "downwind" configuration, where the tower is in front of the turbine, with respect to the wind direction. The unsteady wake shed by the tower and nacelle impinges on the turbine blades causing even further unsteadiness and potentially higher noise and vibration. This simulation was conducted with the enhanced OVERFLOW code.

focusing on is implementing advanced turbulence simulation methods that actually capture some of the scales of turbulence rather than just statistically modeling it all."

Many of the techniques the team employs were originally developed for rotorcraft but are being extended to wind turbines. Rotorcraft is a term that includes a broad spectrum of rotating blade concepts, says Smith, and includes helicopters, tiltrotors, and ducted fans, to name a few.

"Wind turbines have their own set of uncertainties beyond helicopter applications. The blades rotate at tip Mach numbers that are much lower than what are encountered in conventional rotorcraft applications. Wind turbines are also more susceptible to crosswinds and atmospheric turbulence. In addition, their overall operational emphasis is not completely comparable to a helicopter rotor," she says.

Conquering the problem

The team is placing large eddy simulation (LES) methods into classic computational fluid dynamics (CFD) Reynolds-averaged Navier-Stokes (RANS) codes to see if they can more accurately model the physics than what is currently possible with the original turbulence models. The team is modifying two NASA simulation platforms currently used by the wind and rotorcraft industries, OVERFLOW and FUN3D, in order to better account for some of the dominant sources of aeroacoustically generated noise, such as turbulence-induced and blade-vortex-induced noise.

"Whereas the RANS models usually can pick up the gross features, if there is a lot of turbulence involved—a lot of flow separation—then they miss a lot of the secondary and tertiary features that can be important for performance, for vibration, and also for noise," Smith explains.

The team is also investigating the efficiency and accuracy of combining LES and adaptive mesh refinement (AMR) methods in the turbine wakes. Blades rotating against the stationary tower and nacelle—the housing for the gears and dynamo—generate a very dynamic and turbulent wake dominated by powerful tip vortices and separated flow closer to the center. This dynamic nature often means there are regions of the wake with either too much or too little grid resolution just for an instant, increasing the computation time or degrading the results. Linking LES with adaptive meshing, refining, and coarsening focuses computational power where and when it is needed. This task won't be easy; adaptive meshing presents many complications, such as feature detection and load-balancing. But, once these difficulties are overcome, the outcome will be a better result at a lower price, according to Christopher Stone, a local small-business subcontractor of Computational Science and Engineering (LLC) and member of Smith's Georgia Tech team.

OVERFLOW is a structured grid methodology, whereas FUN3D is unstructured. The research and development involving the structured grid methodology is being performed by Stone while the unstructured research is being carried out by Smith and Eric Lynch, an aerospace engineering graduate student. Lynch's work with the unstructured methodologies will be the basis for his Ph.D. dissertation.

The team is running their simulations on NCSA's Mercury cluster. They tested on Cobalt and briefly on Abe, looking at porting performance, but given the structure of the codes the best throughput is obtained using Mercury at this time. The team is also investigating program optimizations and possible restructuring needed to efficiently port to the newer, more powerful systems and will be assisted by the NCSA Advanced Support Program this year.

Other factors

The rotor wake plays an important role, so the team is also looking at how well the CFD models are capturing the wake because the importance of the wake on the loads, as well as the noise, is well known. The team is also moving from just modeling the rotor blades to modeling the wind turbine *in situ*, which includes the rotor blades, the tower, and if necessary, the near-field terrain.

"If you are going to look at the physics in depth you need to be able to model all components of the wind turbine. The rotor blades move with respect to the stationary components, and that's a very expensive simulation," says Smith. "So we are also looking at applying actuator disks and actuating blades, where we model just the blades' impact as a source field and not the actual blades. We couple the CFD code with a structural dynamics code that tells us where these blades are moving in space using the aerodynamic loads from the CFD model. This process is iterated until the loading and blade motion is periodic. These reduced rotor models, I think, are going to be useful when you're trying to get a gross approximation of the interaction of the wind turbine wakes with other features, such as a farm building or a mountain or in a wind farm. This concept will take a lot less time to analyze, and I think it's important that we have that capability."

Finishing touches

The final step for the team is examining the acoustics. By taking the methodology they developed and coupling it with known rotorcraft acoustic prediction methods, they believe they can determine what the acoustics are, both the higher-frequency noise that they can easily see in the models, and also the lower-frequency noise.

Smith and Stone say they are about midway through their processing cycles and tool development. But their results so far, which include improved turbulence modeling and unsteady low Mach number preconditioning (improving numerical accuracy and efficiency for low Mach number flows), are already garnering attention from other researchers, manufacturers, and government agencies. When completed, their tool will allow manufacturers and others working with wind turbines and wind farms to develop machines and installations that have improved aeroacoustics as well as increased operating efficiencies. □

Project at a glance

Team members

Marilyn Smith
Christopher Stone
Eric Lynch

Funding

National Science Foundation

More information

www.ae.gatech.edu/~msmith
www.computational-science.com

Access online

www.ncsa.illinois.edu/News/Stories/Windturbines

The perfect pair

By Barbara Jewett

Researchers rely on NCSA's Mercury to overcome a major barrier in shrinking capacitors for microelectronics use.

A SUPERCOMPUTER IN YOUR POCKET? Probably not. But thanks to today's high-performance computing, the electronic devices you'll carry in your pocket in future will most likely be smaller and have larger, more powerful memories than the ones you're toting around now.

That's because advances in supercomputing combined with advances in science enabled a California research team to identify a solution to a key challenge faced in miniaturizing devices—shrinking the size of the capacitors. A capacitor in its simplest form consists of two conducting plates separated by an insulating layer called a dielectric. In electronic circuits they have many uses, such as providing barriers to prevent current leakage, storing charge, or storing data in memory applications.

Capacitors are often the largest component in the circuits found in microelectronics. But reducing capacitor size for use in ever-smaller electronic devices is hampered by depolarization effects arising from the electrode-film interfaces. This results in reduced interface capacitance—a "dead layer" at the surface that reduces overall performance.

Experimental colleagues brought the dead layer problem to the attention of computational scientists Massimiliano Stengel and Nicola Spaldin in the Materials Department at the University of California, Santa Barbara, and David Vanderbilt in the Department of Physics and Astronomy at Rutgers, The State University of New Jersey. With increasingly sophisticated methods for growing films and interfaces, "new experimental data was causing researchers to revisit long-held assumptions about the nature of this dead layer problem," Spaldin says. Her team "got involved because it seemed like an intriguing problem that we could directly contribute to—what are the fundamental limitations associated with such interfaces, and how much of the experimental limitations are due to defects or imperfect growth? In a calculation we can make a perfect interface without any defects and see what the intrinsic limit is for the behavior."

The team used first principles density functional theory calculations to prove that an intrinsic dead layer actually exists, then to study its origin. They calculated specifically the response of all of the atoms in a model capacitor to an applied electric field, then analyzed the dielectric response—the amount of polarization per applied electric field—locally across the structure. "In late 2006 we saw our first computer images of a 'dead layer': A huge suppression of the dielectric response at an ideal interface," says Spaldin. "While we could see what was causing it, and that it really was intrinsic to the system, it's taken us since then to figure out how to fix it."

Like a miniature industrial facility, tiny capacitors on a processor chip carry out a variety of different tasks for the CPU.

Computer chemistry

What the team did to discover the fix, says Spaldin, was "almost like a chemistry experiment" except it was conducted via supercomputer. The project used over 100,000 hours of computing time, on NCSA's Mercury and also at the San Diego Supercomputer Center. Without current compute resources, she says, they would not have been able to take on this research.

"The ability to do this is something that is fairly recent, both in terms of the availability of the tools and techniques and the availability of computer resources," says Spaldin. "Even with the most sophisticated algorithms, this was still a big number crunch."

The team made repeated calculations with varied combinations of different metals and different ferroelectrics (materials with a spontaneous electric polarization that can be reversed with an electric field). The calculations utilized a density-functional theory code that the team customized with some methods extensions in order to constrain the electrical boundary conditions, allowing them to apply an electric field to the system or to constrain the internal polarization. Analyzing the results, the first thing the team noticed was surprising: a strong dependence on the details of the chemistry of the metal/ferroelectric interface. They then spent nearly another year exploring why particular combinations of chemistry responded as they did.

The next step

The team determined computationally that using barium titanate for the ferroelectric and platinum for the metal essentially reversed the effect of the dead layer, increasing the overall capacitance. The next step is for an experimental group to validate the team's work in the laboratory.

"It used to be thought that there was really a fundamental size limit below which you couldn't go, because your ferroelectric would stop being ferroelectric because of this dead layer and would just give up," Spaldin says. "What we've found is that with the barium titanate/platinum combination—even for just one layer, just one unit cell—the barium titanate stays ferroelectric."

If the work holds up experimentally, the potential then exists to make thin-film ferroelectric memory chips that are smaller than anything currently on the market and capable of holding significantly more data. This could make ferroelectric memory more competitive with magnetic memory. The team hopes their results motivate experimental scientists to further explore controlling the structure and termination of perovskite/simple metal interfaces, yielding additional discoveries in engineering the electrical properties of thin-film devices.

"There's so much else going on in integrated circuits that may end up influencing whether our work gets adopted or not, rather than the basic physics of the interface," Spaldin says, noting that it often takes years for new discoveries to be successfully incorporated into products.

Even if their capacitor isn't adopted by industry, the team established some major theoretical groundwork which was published in *Nature* earlier this year. In particular, they are very excited about the capability they were forced to develop in order to answer the dead layer question. They believe the capability of controlling the electric field or defining the electrostatic boundary conditions in a density-functional theory calculation is something that is going to be widely applicable to a variety of research problems.

"Any time you want to model a material in a realistic device situation, you need to include metallic electrodes, which means you will have an interface between the metal and your material. Then in order to be able to make a physically meaningful calculation you need to be able to apply electric fields and/or control the electrical boundary conditions within the calculation. Our development of the tools to do this could turn out to be the most significant outcome of this work. We now have a tool—the theory community now has a tool—that can be applied to other combinations of materials where there are open questions and problems to solve. "

Moving forward

The next direction for the team is also on the theoretical front. They'll explore combining the application of magnetic fields and electric fields in their calculations, allowing them to explore a whole new capability of what is called magneto-electric response.

"We'll be looking at how electrical properties change with magnetic fields and vice versa, as well as whether we can get coupled properties by applying both types of fields simultaneously," says Spaldin. "Now that we have this capability, that's the next frontier we're playing with." □

Project at a glance

Team members

Nicola Spaldin
Massimiliano Stengel
David Vanderbilt

Funding

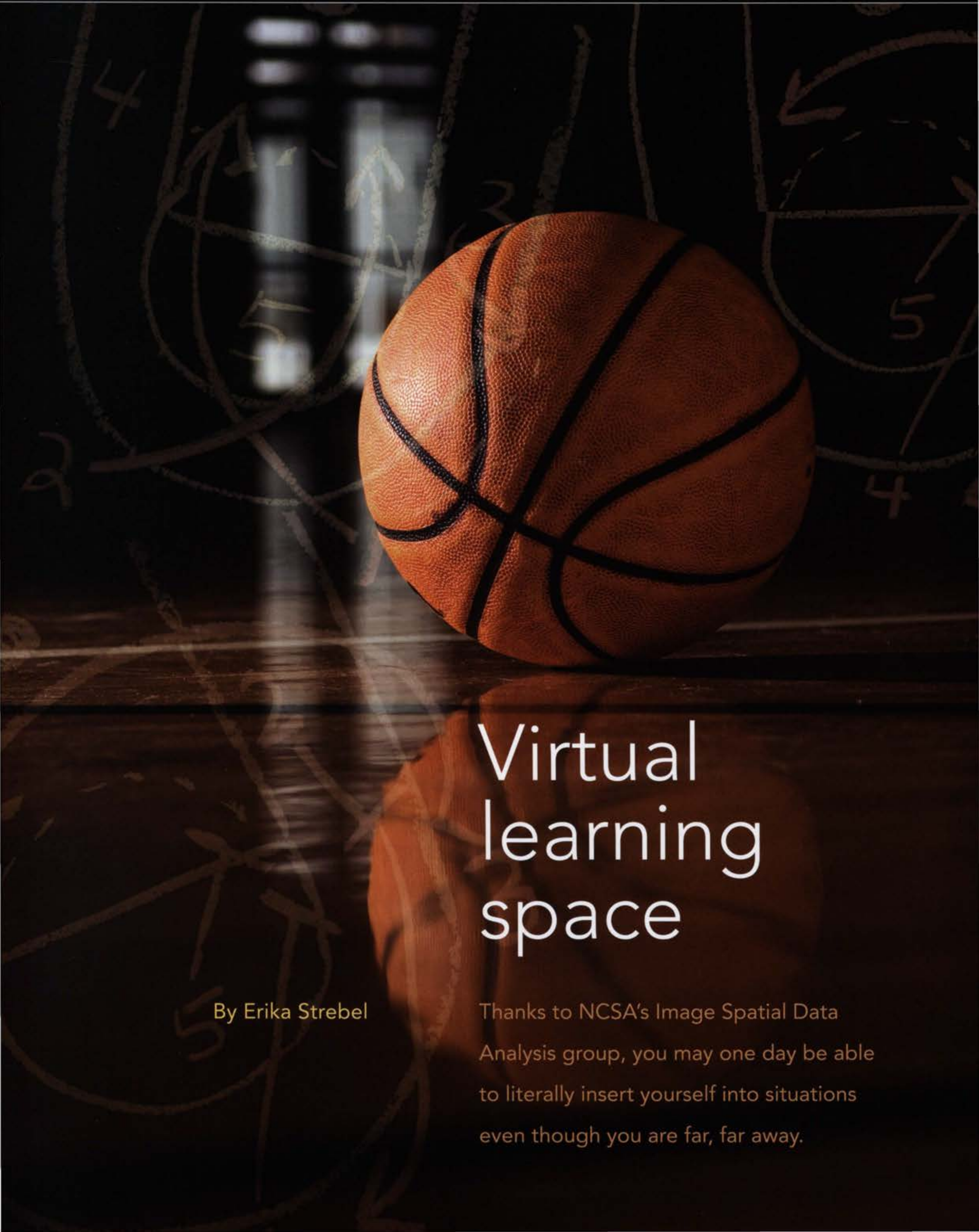
Department of Energy's SciDAC
Office of Naval Research

More information

www.mrl.ucsb.edu/~nicola/

Access online

www.ncsa.illinois.edu/News/Stories/Capacitors



Virtual learning space

By Erika Strebel

Thanks to NCSA's Image Spatial Data Analysis group, you may one day be able to literally insert yourself into situations even though you are far, far away.

1 The team uses special software to help design and deploy the camera and lighting configuration for each tele-immersive system. Software is also used to calibrate cameras for optimal results.

2 Unlike the 3D polygon models people see in video games or in digitally animated films, this virtual environment records real-time actions. Since the system relies on real-time imaging, no one needs special equipment to do complicated 3D reconstruction.

THERE ARE MANY WAYS of communicating with people who aren't in the same area. You can use a telephone or e-mail to talk to a relative living thousands of miles away. Talk show hosts sometimes use Skype to chat with interviewees who couldn't make it to the set. You can listen to a live lecture or seminar online. But learning physical skills, like basketball, is more difficult since these technologies do not allow an instructor and a student who are geographically separated to physically interact.

NCSA's Peter Bajcsy wants to push those limits. He and his team are collaborating with various units at the University of Illinois at Urbana-Champaign—the computer science and electrical and computer engineering departments, as well as disability resources and educational services—and University of California, Berkeley to develop a way to digitally clone people in remote areas into the same virtual space and allow them to physically interact in real time.

Putting reality into a virtual space

The team constructed a system of cameras and displays that capture, transmit, and display three-dimensional movement in real time. Several digital camera clusters consisting of visible and thermal spectrum cameras, and multiple large LCD displays surround a defined physical space where someone will be learning complex movements or physical activities, like wheelchair basketball.

The camera clusters are placed on tripods and the LCD displays are mounted on TV carts so the system is portable. Three-dimensional information is extracted from the images those cameras acquire and rendered in a virtual space.

With the help of various software, the system makes 3D data in real time available to remote machines through the Internet. LCD displays allow users to see their own digital clones and the clones from remote sites together, and move their bodies in response to the images on the screen.

Bajcsy, the team's leader and head of the image spatial data analysis group at NCSA, calls this a "tele-immersive environment" because a user can be immersed with another user at a remote site and communicate in 3D and in real time. Unlike the virtual reality people see in video games or in digitally animated films, these virtual environments record real-time actions.

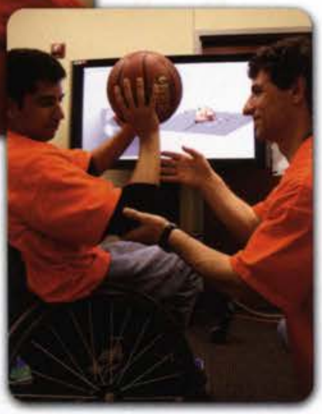
"It's a virtual environment that is the product of real-time imaging, not the result of programming 3D CAD models." Bajcsy says. "Nobody has to be supplied with equipment to enable imaging and 3D reconstruction. The only thing you might have is some kind of controller, like a Wii controller, so you can change the view angle of the data you see."

In 2007, Bajcsy and his team started working with groups of wheelchair basketball players to test the tele-immersive system. During these experiments, wheelchair basketball coach Michael Frogley and his students work on basketball moves and wheelchair maneuvers.

"I really have to praise the wheelchair basketball players," said Bajcsy. "They are just really fun to work with! They are always interested in trying the new technology, although the technology might be frustrating."

Deploying a tele-immersive system

Before deploying the system, a user would need recommendations where to place clusters of cameras. Bajcsy's team designed a simulation framework that allows users to input the amount of money available, the type of activity they want to learn, the dimensions of the space they want to use, and information



3 The remote capabilities of the system allow multiple sites to interact in the same virtual environment—for instance, a coach monitoring practice from a remote location or a player being able to see himself from multiple angles in order to better hone his skills.

Project at a glance

Team members

Peter Bajcsy
Rob Kooper
Suk Kyu Lee
Rahul Malik
Kenton McHenry
Hye Jung Na
Andrew Spencer

Funding

National Science Foundation

More information

isda.ncsa.uiuc.edu

Access online

www.ncsa.illinois.edu/News/Stories/WheelchairBB

about lighting in that space. The framework will determine the number of cameras the group should purchase and where to position those cameras.

The NCSA team also devised a special code that allows the camera clusters to be calibrated in terms of color consistency and geometric locations/orientations once the camera clusters are placed.

Tweaking the system

Over the course of the project, Bajcsy and his team have made various adjustments to the system.

"As we were starting to build the system, we immediately noticed the system had some robustness issues with respect to illumination," Bajcsy says. "The system would not perform well when illumination would change or objects would not be different from the background."

In order to fix this issue, the team introduced thermal-infrared cameras to the system, allowing the system to identify things that are warmer or cooler than the ambient temperature in the environment. As a result, the system can detect the foreground regardless of what subjects are wearing or whether they cast shadows, said Bajcsy.

But there are more challenges ahead.

"The system is very dynamic," said Bajcsy. "Bottlenecks are shifting to different places in the system as you replace technology or technology works better."

The team is now trying to fix a networking and data transmission problem. A single camera cluster generates about 460 megabytes of data for every second of real-time footage, which is just under half of a gigabyte of information. But only one gigabyte per second of total bandwidth is available. This poses a problem because a system that employs 10-20 cameras would easily surpass that bandwidth, says Bajcsy.

"We are working very closely with Professor Klara Nahrstedt's group in the computer science department," says Bajcsy. "Their expertise is in networking, so we'll be relying on them for the right protocol."

He says the NCSA team is also collaborating with electrical and computer engineering departments at the University of Illinois and UC Berkeley to compress the 3D information, and to consider alternative ways of representing data collected from the cameras.

Moving forward

Bajcsy and his team are continuing to improve their system to meet the needs of the wheelchair basketball community.

"If we could build a system so that it works robustly and can be deployed in the gym where they practice every day, then it would have tremendous value for them," says Bajcsy.

The NCSA team has also been working on adding a replay feature that would allow a user to replay a previous session while in the virtual space.

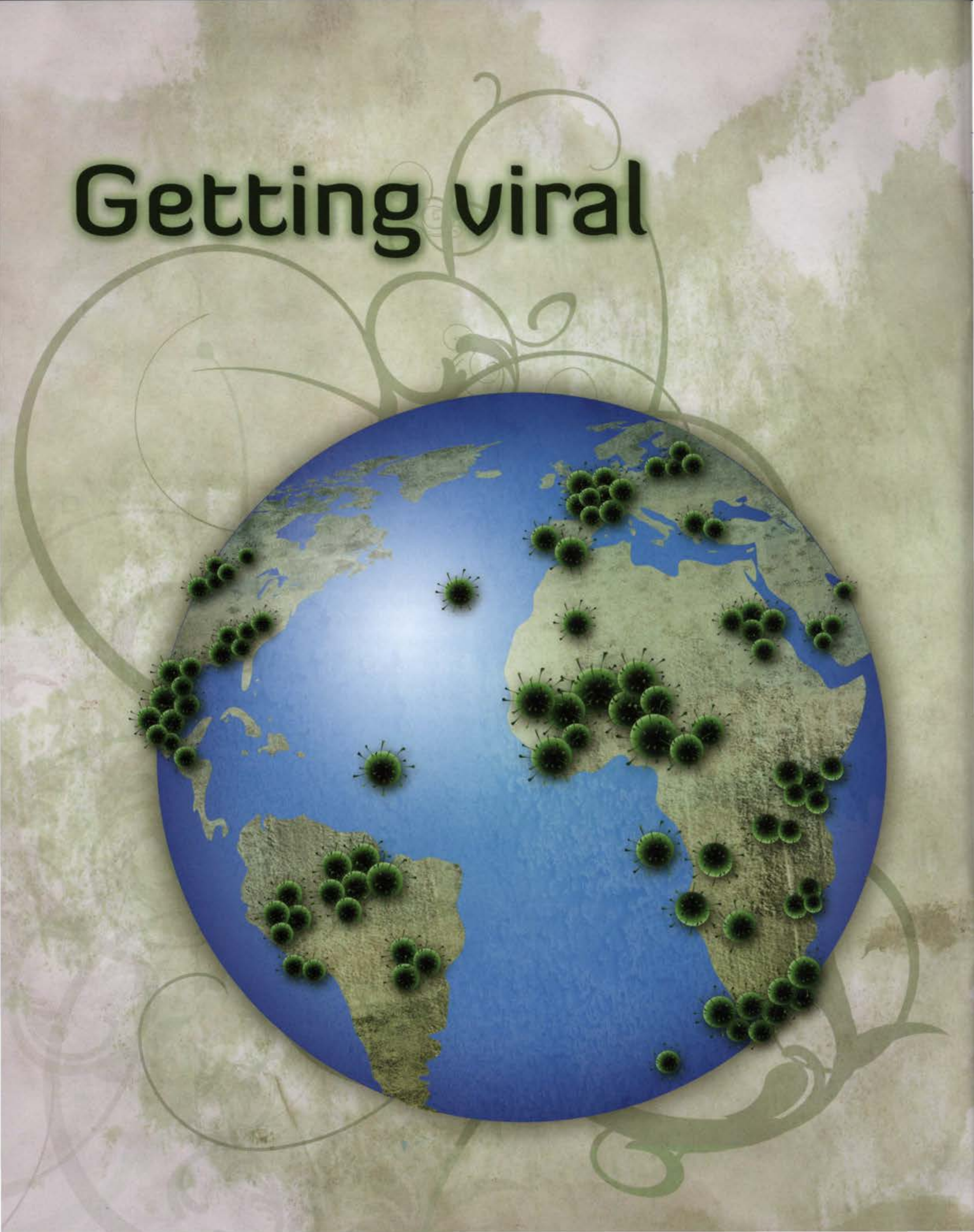
"You can actually exercise next to yourself and say, 'Oh, I see. I was making that mistake,'" said Bajcsy.

The ultimate goal is to construct a system that costs less than $50,000. Current models on the market cost at least half a million dollars and focus primarily on head movements. However, Bajcsy says commercially available technology is still not advanced enough to make the system more portable and resilient.

He also hopes to be able to connect four to five remote sites at NCSA and the computer science department so that his team can demonstrate the scalability of the system.

"As we demonstrate that the system is really working," he says. "I'm looking for other communities who can take advantage of the technology." □

Getting viral



By J. William Bell

Some early prospective users of Blue Waters will build computing code for global epidemic models.

INFECTIOUS DISEASES can have very different characteristics. Measles strike in related waves over the course of decades. Any given flu strain tends to peter out in a year. A flu victim is thought to infect about two additional people, a measles victim as many as 14.

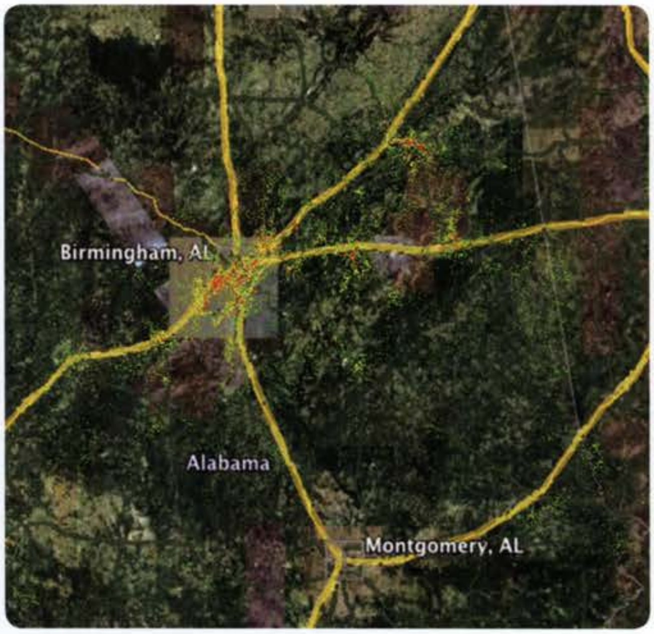
But any disease that passes person-to-person shares at least one common characteristic: Its spread can be modeled using a supercomputer.

Those models serve two key purposes—policy planning and emergency response.

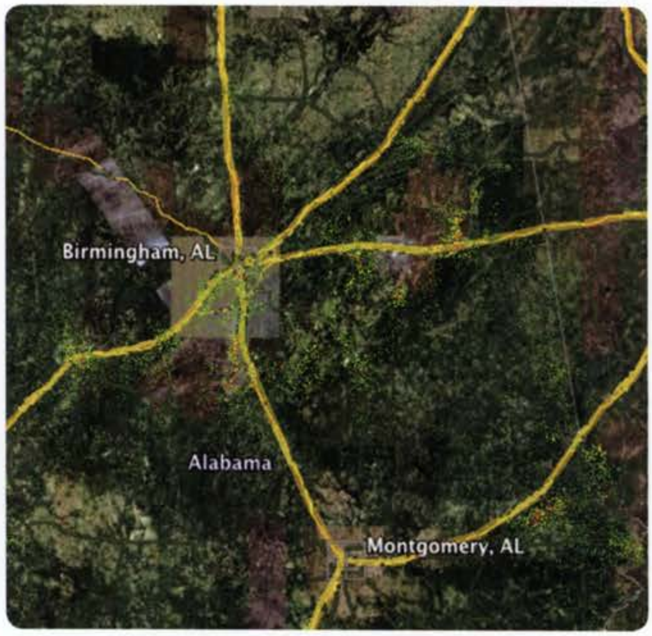
"In the planning world, we work with policymakers to design studies of particular outcomes," says Virginia Tech's Keith Bisset. Months of planning, collaboration, and modeling might go into strategies for what a city, county, or entire country might do when facing a disease outbreak.

"But now we also have tools that allow for a quick turnaround. We can do a situational assessment that shows them what a particular [outbreak] might look like tomorrow or next week as it unfolds. They describe the situation, and we can tell them the outcomes of various interventions," he says.

DAY 72 NO INTERVENTION



DAY 72 VACCINATED CHILD 100%



Comparison of one day from a simulation of pandemic influenza in Alabama from Virginia Tech's EpiSims code. The color of the dots represent the number of infected individuals who live in that geographic area, green for low through red for for high. In the simulation on the left, no intervention was done. In the simulation on the right, all children under 18 were vaccinated with a low efficacy vaccine.

Going global

This spring Bisset and a group from Virginia Tech joined forces with the Pittsburgh Supercomputing Center's Shawn Brown and Douglas Roberts and Diglio Simoni of North Carolina's Research Triangle Institute to win one of the first Petascale Computing Resource Allocations awards.

With that support and with computing time on Blue Waters, they expect to model global epidemics, as well as smaller-scale outbreaks. Instead of looking at a few hundred million people, as the team members do with their current codes, they'll look at more than six billion people.

"There's a natural limit to how big we make the models in terms of the number of people," Bisset says. "Once we're doing every person in the U.S. or every person in the world at one-minute intervals, there's no value to making it bigger."

Making it that big, however, will require a lot of work. The team estimates that a global model on 2,000 processors of a contemporary supercomputer would take about two years to complete. "This is clearly unacceptable," they said in their Petascale Computing Resource Allocations proposal.

Part of the challenge is that a single predictive model is based on what is often thousands of computing runs, each with slightly different parameters representing things like people's social contact and behavior and the different disease characteristics.

In contrast to other supercomputing problems, for example large physics simulations, "the outcome of a single run is not interesting by itself," according to the proposal. "Simulations of infectious disease outbreaks are not run for their own sake, but to investigate specific questions about prevention and mitigation. Answering these questions requires analyzing the interdependent effects of many different parameters."

"The goal is not to answer a single question of what happens 'if'," explains Virginia Tech's Stephen Eubank. "It's to compare. Is intervention A better than intervention B?" In other words, does closing a city's schools have more impact than giving citizens a prophylactic medication against infection? Or, for that matter, does doing either or both have enough of an impact to justify the social and economic costs involved?

The team will focus on optimizing their code and scaling it to run on Blue Waters' hundreds of thousands of processors. That global model that would take years on today's supercomputers? They hope to complete it in a couple of weeks on Blue Waters.

"Overall time-to-solution is the measure of effectiveness. Today, many policymakers are forced to use inaccurate tools in place of accurate, but slower, tools," according to the team's proposal. With Blue Waters, they hope to change that. □

SPACES

SPACES, the code a Virginia Tech team will develop for Blue Waters, is based on their current code called EpiSims. Codes like these are particularly challenging because they simulate disease moving through a set of overlapping social networks—schools, families, and international travelers.

"It's not just local. It's not just global. It's just irregular. People are close in one network, scattered in another. We can't decouple them," says Stephen Eubank, a research professor at Virginia Tech.

But working with the Blue Waters team through the Petascale Computing Resource Allocations program will allow them to:

- break the code into pieces to run over hundreds of thousands of processors.
- develop schemes for automatically balancing the computing load so that parts of the simulation that share data are near one another and can thus pass the data more quickly.
- take advantage of virtualization to move parts of the computation to other processors and memory in Blue Waters, should an individual component fail.

These improvements will be implemented using Charm++, a parallel programming system developed by Sanjay Kale's team at the University of Illinois at Urbana-Champaign. Kale is a computer science professor, an integral part of the Blue Waters team, and a member of the Institute for Advanced Computing Applications and Technologies.

First Blue Waters projects selected

This spring and summer, the National Science Foundation announced the first winners of its Petascale Computing Resource Allocations awards. These research teams will work closely with the Blue Waters project team in preparing their codes to run on the sustained-petascale supercomputer. They'll also be given the opportunity to apply for time on Blue Waters once it comes online in 2011.

NSF plans to select about a dozen teams per year between now and 2011.

"Preparing these codes to run on Blue Waters is absolutely essential to our success," explains Thom Dunning, who leads NCSA and the Blue Waters project. "We're committed to providing sustained-petascale performance on the system, and that means working with scientists now, not in three years.

"It's a very select group, and we're very excited to get started."

Think of them as "The Elite Apps" of the supercomputing set. These are the scientific applications that have made their way through the selection process. The computing codes that have passed muster with their peers. The codes that will get special attention. The teams that are ready to make the most of the most powerful supercomputer in the world for open scientific research.

As of press time, these projects had been chosen to work with the Blue Waters team through the National Science Foundation's Petascale Computing Resource Allocations. More will be added throughout the next three years.

- **Formation of the First Galaxies: Predictions for the Next Generation of Observatories**
  Brian O'Shea, Michigan State University
- **Simulation of Contagion on Very Large Social Networks with Blue Waters**
  Keith Bisset, Virginia Tech; Shawn Brown, Carnegie-Mellon University; Douglas Roberts, Research Triangle Institute
- **Lattice Quantum Chromodynamics on Blue Waters**
  Robert Sugar, University of California, Santa Barbara
- **Super Instruction Architecture for Petascale Computing**
  Rodney Bartlett, University of Florida
- **Peta-Cosmology: Galaxy Formation and Virtual Astronomy**
  Kentaro Nagamine, University of Nevada, Las Vegas
- **The Computational Microscope**
  Klaus Schulten, University of Illinois at Urbana-Champaign

HYDROGEN HARVEST

By Trish Barker

A computational approach and NCSA resources help MIT researchers better understand the process of manufacturing hydrogen.

HOW DO YOU HARVEST HYDROGEN? The abundant proton-neutron-electron combo accounts for about three-quarters of the elemental matter in the universe, but collecting a sufficient supply for industrial uses—from the mundanity of fertilizer production to the potential for hydrogen fuel cells to reduce our carbon footprint—requires a manufacturing process.

A common method of manufacturing hydrogen is steam methane reforming (SMR), which combines methane, steam, and a metal catalyst (such as nickel) in a high-temperature environment. The process has been used for many years and has been studied in detail, but there are still gaps in scientists' understanding.

"The problem for all heterogeneous catalysis is something called the 'pressure gap'," explains Wayne Blaylock, a chemical engineering PhD student at MIT. "Experimental observation of these processes is limited largely to instruments that operate at a very low pressure. And industrially, you can't make any money operating at that low pressure, so you will operate at much higher temperature and pressure."

That means that the experimental picture doesn't match how the process occurs in the real world. That's why the research team led by Blaylock's advisor, MIT chemistry professor William Green, adopts an *ab initio* computational approach to model the thermochemistry of SMR under industrial conditions. The goal is to obtain a better understanding of the surface pathways and reactions that control SMR in order to design new catalysts and to control the by-products of the reaction (such as catalyst-clogging carbon).

Their analysis of the key Ni(111) catalyst surface was presented at the spring 2008 meeting of the American Chemical Society.

Unexpected pathways

Using density functional theory (DFT) and statistical thermodynamics, the researchers have developed a detailed model of the intermediate species and transition state behavior occurring in SMR over Ni(111), the most predominant and thermodynamically stable phase of the nickel catalyst. Their calculations include the high temperature (800 degrees Celsius) and pressure (10 bar) that are realistic for hydrogen manufacturing, and they investigated 36 reactions involving 26 species.

The team performed flux and sensitivity analysis on their kinetic model to determine which reaction pathways are dominant and which steps control the rate of the reaction on the Ni(111) surface.

Their work relied on the Tungsten and Abe clusters at NCSA, in addition to a small computer system in their lab at MIT.

"We're just now getting to the point where we can do this type of modeling; in the past five years or 10 years, the hardware has become more capable of handling this sort of computation," Blaylock says. "Because we want to look at all these different pathways, because we don't want to make assumptions about what is important, we have to look at many species, many reactions on many catalyst surfaces. We looked at every feasible combination of one water and one methane molecule on the surface. We didn't just look at one pathway, we looked at many reaction pathways that could lead to the desired products.

"And that's what drives our reliance on the supercomputing resources."

The researchers found that the steps limiting the rate of the overall reaction were the reactions of CH with O and OH to form CHO and CHOH; the dominant pathway was through CHO.

"Most people would assume that the dominant pathway on the surface would be through a carbon and an oxygen, forming CO," Blaylock says. "But what we found through our microkinetic modeling is that there were other pathways that were more favorable. "It turns out that the C species is very unstable on the Ni(111) surface, and that instability makes reactions involving it kinetically unfavorable.

"Really the only way of realizing just how unstable this species is was computation," Blaylock says. "The important message to take away is that this sort of comprehensive modeling can provide insights that might be contrary to popular assumption or popular belief.

"Computation can really bring the surface into view, where before you simply couldn't see it using available experimental techniques."

Of course, experimental techniques are growing more accurate as well, providing the potential to validate the computational model with experiment and to guide experiment with computational insights.

"What that really means," Blaylock says, "is pairing experiment and computation and driving toward a unified microkinetic model. The amount of information we are able to obtain will just continue to increase from experimentation and computation in connection."

Catalysts and carbon

Ni(111) is just one aspect of the nickel catalyst; there are other nickel step sites that the team plans to model as well, determining their surface energies and reaction barriers and constructing a model that combines all of the nickel facets.

"We've only performed comprehensive work for the Ni(111) surface, but we hope to do a more unified model of various catalyst facets going forward," Blaylock says. "This will give us a better idea of what a real catalyst might do under real conditions."

Determining which steps limit the rate of the reaction provides a target for catalyst development. "If you know the bottleneck, you can design a new catalyst to address that," Blaylock explains.

The researchers are investigating nickel alloys, such as nickel doped with a small amount of silver. So far, a catalyst in which one of every four surface atoms is silver seems to slow the SMR process by an order of magnitude. That doesn't seem like a desirable result, but if a slower reaction results in less carbon formation, that trade-off might be worthwhile.

That's because carbon formation is the bane of hydrogen production. Carbon can build up, encapsulating the catalyst and preventing it from reacting with the methane gas. That's usually just a temporary problem that can be solved by stopping the flow of methane, pumping in oxygen, and letting the carbon burn away in the already high heat required for SMR. But a more serious form of carbon buildup, called whisker formation, can actually crush the catalyst. In the experimental membrane reformers that might someday supply pure hydrogen for fuel cells, this could be disastrously expensive. Finding reactions that reduce carbon creation is therefore another important target for the researchers. □

Project at a glance

Team members

Greg Beran
Wayne Blaylock
William Green
Teppei Ogura

Funding

StatoilHydro
Norwegian Research Council
National Science Foundation Graduate Research Fellowship Program

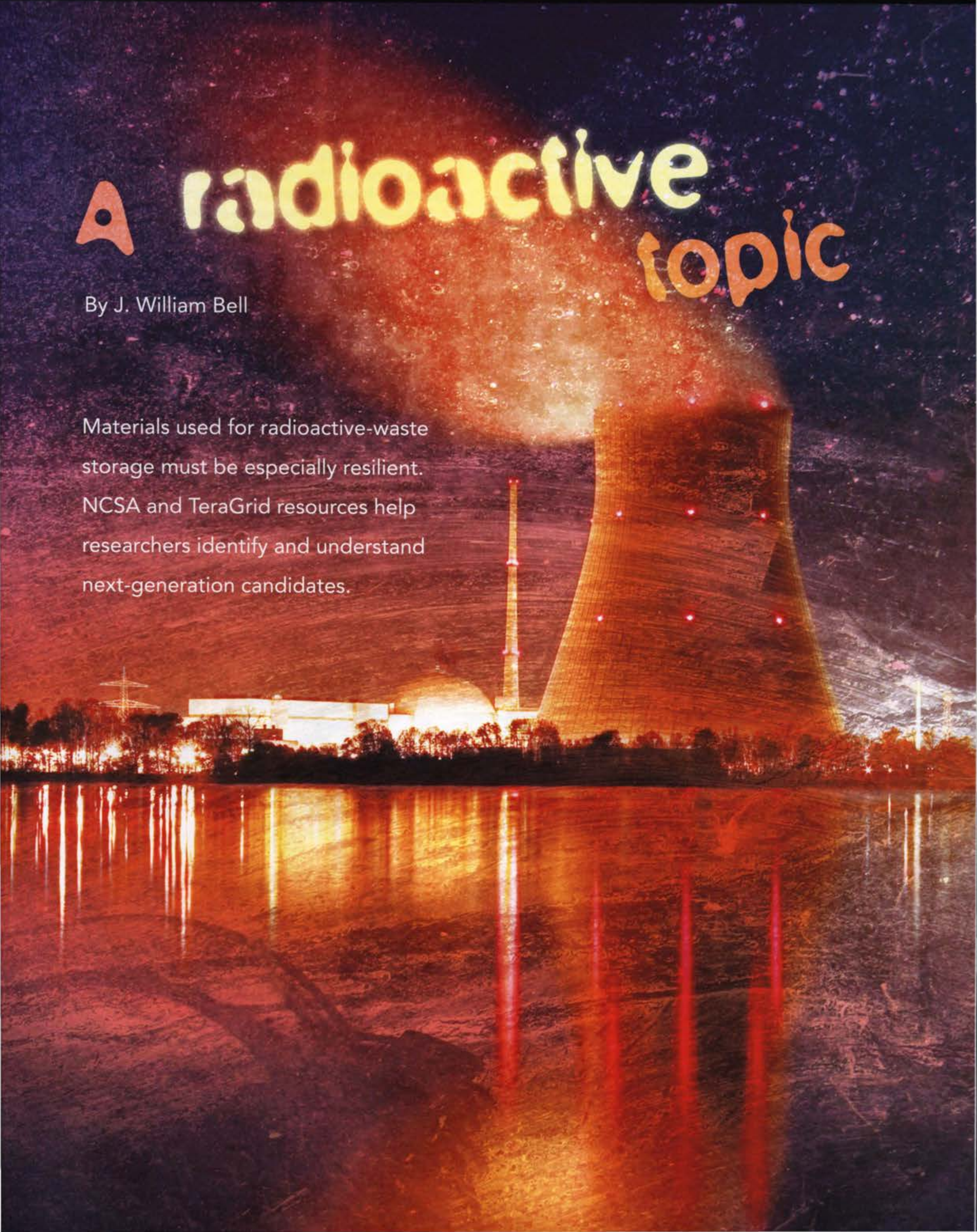
Access online

www.ncsa.illinois.edu/News/Stories/hydrogen_harvest

A radioactive topic

By J. William Bell

Materials used for radioactive-waste storage must be especially resilient. NCSA and TeraGrid resources help researchers identify and understand next-generation candidates.



SOME 60,000 TONS of high-level radioactive waste is being stored in the U.S., according to a 2006 report from U.S. Geological Survey scientists. Coming largely from nuclear power plants and retired nuclear weapons, it resides at more than 100 temporary sites around the country.

The containers used today aren't viable candidates for long-term storage. They're 100-year solutions to 100,000- or million-year problems, based on "a special glass that cracks. Not very good for long time periods," explains Jianwei Wang, a post-doc at the University of Michigan.

Finding the right material in which to store the waste underground over the course of millennia is a great challenge.

As part of a team from Michigan and Rensselaer Polytechnic Institute, Wang is using TeraGrid resources to investigate pyrochlores. These minerals show natural resistance to radiation and can be altered to make them hundreds of times more resistant to the structural defects that crop up under the extreme irradiation and pressure.

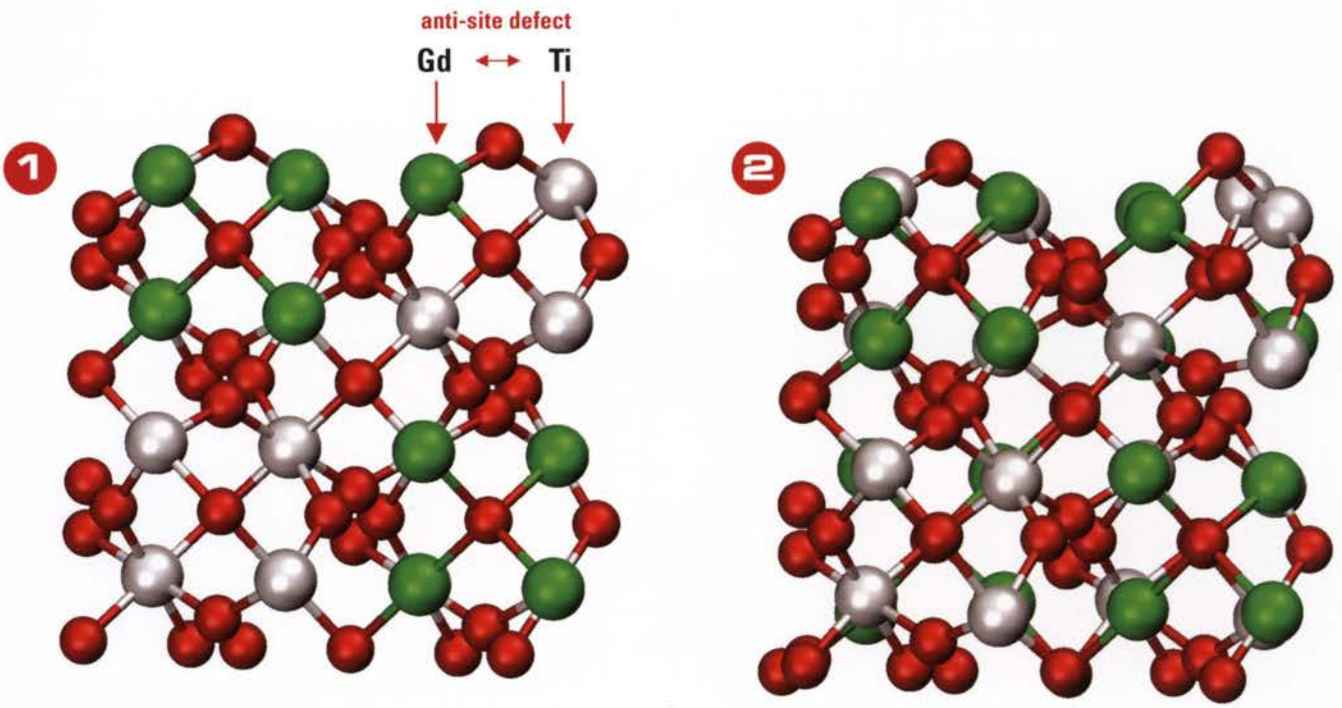
With NCSA's Cobalt system, the team is showing that the performance of these materials in extreme environments is directly related to the energies at which defects form. They also use the Kraken system at Oak Ridge National Laboratory.

For example, their studies show that two pyrochlores—gadolinium titanate and gadolinium zirconate, in which titanium can be exchanged with zirconium—display dramatically different behaviors under irradiation and pressure. Results were published in *Physical Review Letters* in 2008. Modeling the pyrochlores at progressively higher pressures and 1,800 Kelvin showed that the zirconium-based structure could accommodate 1,000 times more defects than the titanium-based structure at pressure up to 20 gigapascals.

The modeling also showed that the number of defects in the zirconium-based structure decreased while those in the titanium-based structure increased as the pressure increased toward 20 gigapascals. These results were presented at the Materials Research Society Fall Meeting in December 2008.

Perhaps counterintuitively, defects at the atomistic scale improve materials' resistance to radiation, according to Wang. "Irradiation induces defects and the accumulation of these defects can lead to disorder in the material. But studies show that irradiation resistance improves in proportion to the atomic disordering tendencies" of the materials.

The team combines their computational simulations with ion beam experiments. Rod Ewing, a Michigan professor who leads the



Irradiation damage starts with defect formations. These show the effect on the surrounding structure by a simple anti-site defect in $Gd_2Ti_2O_7$ pyrochlore. The defect is defined by switching a pair of gadolinium and titanium atoms in the structure, common in most irradiated pyrochlores. A single defect in the pyrochlore induces structure distortions of all 88 atoms in the computational cell, far beyond the atoms immediately surrounding it. The green balls are gadolinium atoms, the white balls titanium atoms, the red balls oxygen atoms, and the sticks bonds between atoms. The red arrows point to initial defect locations.

group along with Michigan's Udo Becker, says the two approaches "work well together. They're intimately mixed."

Experimental findings validate computational findings, and vice versa. Just as importantly, they show the researchers different parts of the whole. "Experiments can look at the gross effect [that radiation and pressure have], but to gain insight into the process itself, we need simulation," Ewing explains.

At the fundamental level, computations show how the free energies of atoms of materials with different chemical structures vary under more and more extreme conditions. Those differences simply can't be observed in the ion-beam experiments.

Overall, this combination of experiment and computing "provides a scientific basis for the next generation of nuclear waste [containers]," says Wang. "The computational part of the effort is important for the success of our projects, and the Teragrid resources are essential for our computational work."

"Not to be immodest, but this is exciting and important science. It allows us to begin to consider ways we can make materials that are more radiation resistant," Ewing says. □

Project at a glance

Team members

Rod Ewing
Udo Becker
Jianwei Wang
Fuxiang Zhang
Maik Lang
Jiaming Zhang
Jie Lian

Funding

Department of Energy
National Science Foundation

More information

www.geo.lsa.umich.edu/relw/groupmembers/ewing/ewing.htm
www-personal.umich.edu/~jwwang/
www.geo.lsa.umich.edu/compmin/

Access online

www.ncsa.illinois.edu/News/Stories/Pyrochlores

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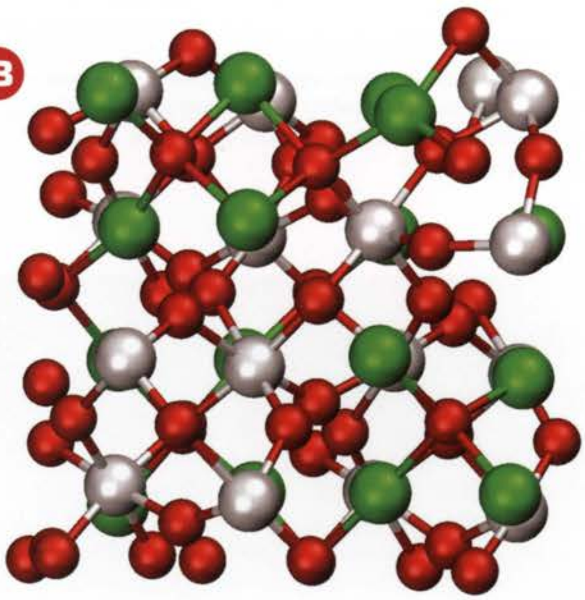
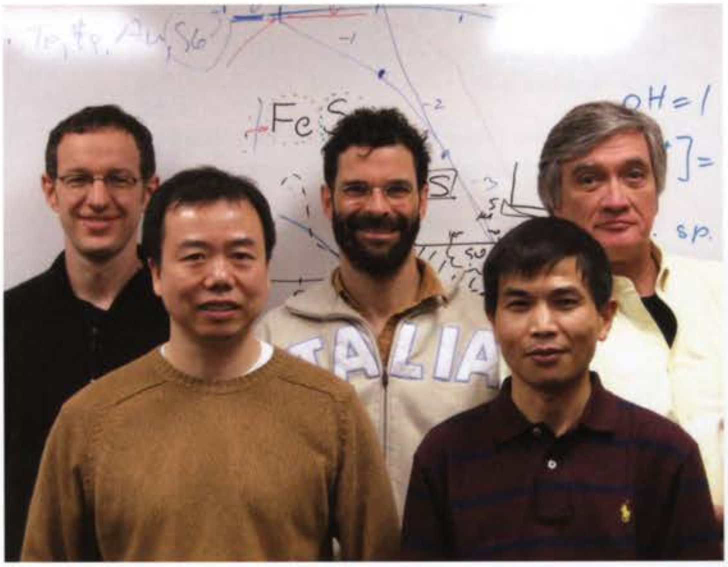




From left to right: Maik Lang, Jianwei Wang, Udo Becker, Fuxiang Zhang, and Rod Ewing.

NCSA researcher receives seed grant

Under the auspices of the Illinois Informatics Institute, the Community Informatics Initiative (CII) will integrate community informatics into various disciplines across the University of Illinois at Urbana-Champaign campus. In April, a CII committee awarded seed grants to nine faculty projects. The recipients will be appointed CII Fellows for 2009-10, collaborating with CII and sharing their work in the CII research series. The fellows include NCSA research scientist Ian Brooks, head of the health sciences group, for "Culture-Sensitive Interface Design for an Endemic Disease Information System" that will develop a malaria tracking data collection system that's compatible with the education level and technology available in certain African countries.

NCSA awards fellowships to Illinois researchers

Seven researchers from the University of Illinois at Urbana-Champaign have been awarded fellowships to pursue diverse collaborative projects with NCSA during the 2009-2010 academic year:

Michael Dietze | **Plant Biology**
Refined estimates of the eastern North American carbon budget: Multi-objective model calibration and data assimilation

Chatham Ewing | **Rare Book & Manuscript Library**
Multi-spectral imaging and analysis of manuscript materials

Yong-Su Jin **Food Science and Human Nutrition**
Optimal strain design for the production of ethanol from renewable biomass through computing elementary flux modes using a genome-scale stoichiometric model

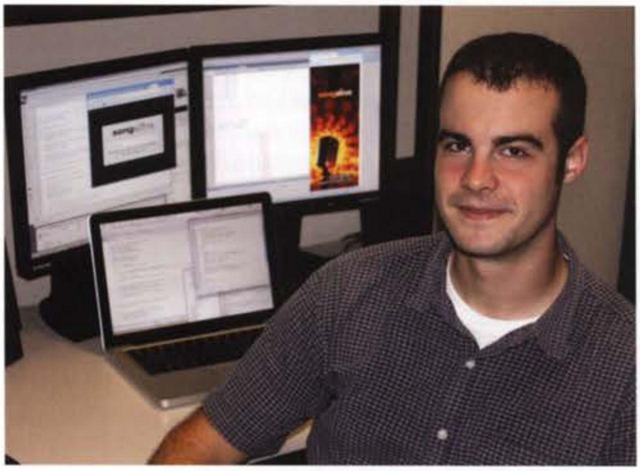
Steven S. Lumetta | **Electrical and Computer Engineering**
Enhancing GPU-based supercomputing through workload and communication optimization

Jian Ma | **Bioengineering**
Algorithms and tools for mammalian genome reconstruction analysis

Junho Song | **Civil and Environmental Engineering**
Rapid decision support for hazard responses by cyberenvironment of urban infrastructure networks

Jacob Sosnoff | **Kinesiology and Community Health**
Accelerometery in wheelchair propulsion

For more information on NCSA fellowships, including abstracts providing more details on the 2009-2010 projects, see:
fellowships.ncsa.illinois.edu



NCSA student employee on winning entrepreneur team

SongAlive, a website that allows musicians around the world to collaborate remotely on songs using audio tracks, was deemed the most fundable venture of the seven teams that made the finals of the V. Dale Cozad New Venture Competition at the University of Illinois at Urbana-Champaign in April. The winning team included August Knecht, a senior in computer engineering and a long-time NCSA student employee.

As first-place finisher, the SongAlive team qualified for iVentures 10, a 10-week summer program to help develop the idea into a working product. Participation in the program is valued at more than $25,000. The team hopes to launch a public version of their website by year's end.

Workshop promotes accelerator use

NCSA recently hosted a three-day workshop, supported by the National Science Foundation, that brought together more than 100 researchers and students in geosciences, chemistry, and astronomy from as far away as Australia and Israel. The workshop was designed to help researchers with some experience in using accelerators such as the Cell processor and graphics processing units (GPUs) advance to the next level of productivity in achieving their scientific goals. Participants were separated into their respective fields of research toward the end of workshop, where they heard from colleagues and exchanged ideas.

The workshop was organized by Robert Brunner, a University of Illinois at Urbana-Champaign astronomy professor, Stanford University chemist Todd Martinez, and NCSA's chief science officer Bob Wilhelmson, an atmospheric scientist.

For workshop presentations and posters see:
www.ncsa.illinois.edu/Conferences/accelerators/agenda.html

New lab focuses on petascale algorithms, software

The University of Illinois at Urbana-Champaign and France's Institut National de Recherche en Informatique et en Automatique (INRIA), recently formed the Joint Laboratory for Petascale Computing. The Joint Laboratory will be based at Illinois. Co-directed by Marc Snir, a computer science professor at Illinois and one of the principal investigators on the Blue Waters project, and INRIA's Franck Cappello, the laboratory will include researchers from INRIA, Illinois' Center for Extreme-Scale Computation, and NCSA.

Much of their work will focus on algorithms and software that will run on Blue Waters and other petascale computers. Early focus areas will include modeling and optimizing numerical libraries, fault-tolerance research, and novel programming models, which allow scientific applications to be updated or reimagined to take full advantage of extreme-scale supercomputers.

INRIA, the French national institute for research in computer science and control, is dedicated to fundamental and applied research in information and communication science and technology, and also plays a major role in technology transfer. The Center for Extreme-scale Computing, part of Illinois' Institute for Advanced Computing Applications and Technologies, focuses on the development of applications and technologies that will help scientists and engineers realize the full potential of future supercomputers.

For more information on the Joint Laboratory, see:
jointlab.ncsa.illinois.edu

NCSA researcher wins NSF CAREER award

The National Science Foundation announced in June that Shaowen Wang won a CAREER award. Wang is an assistant professor of geography at the University of Illinois at Urbana-Champaign and a senior research scientist at NCSA.

The five-year award will support the development of a next-generation Geographic Information System (GIS) framework, called CyberGIS. The new framework will allow geospatial analyses that are markedly more complicated than today by running them over distributed networks of parallel computers like those supported by NCSA. GIS is widely used in a variety of fields, including geography, environmental resource management and impact assessment, urban planning, archaeology, mapmaking, and the humanities and social sciences.

Wang is the founding director of the CyberInfrastructure and Geospatial Information Laboratory at Illinois and runs the TeraGrid GIScience Gateway project.

The CAREER program offers NSF's most prestigious awards in support of junior faculty who exemplify the role of teacher-scholars, allowing them to build a firm foundation for a lifetime of leadership in integrating education and research.

IACAT expands accelerator cluster

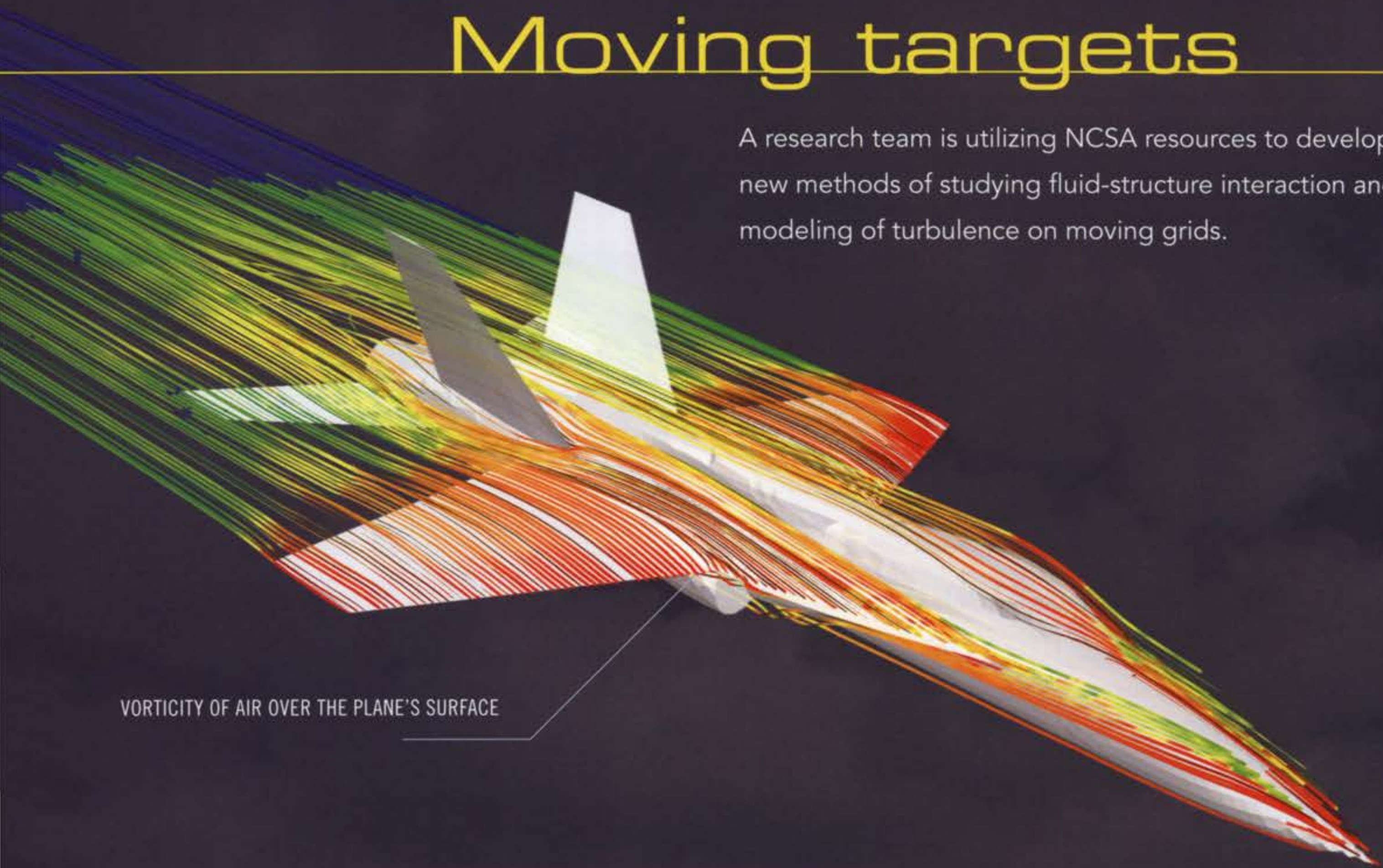
The Institute for Advanced Computing Applications and Technologies (IACAT) at the University of Illinois at Urbana-Champaign has doubled the size of its accelerator cluster from 16 to 32 nodes. Each of the 32 compute nodes is matched with one NVIDIA Tesla S1070 containing four GT200 GPUs, each with 4 GB of memory. The cluster also includes 11 Nallatech H101 PCIX FPGA accelerators, and was recently upgraded with a 2GB/sec InfiniBand connection. NVIDIA donated the Tesla units to Illinois electrical and computer engineering professor and IACAT researcher Wen-Mei Hwu.

The cluster is used for electrical and computer engineering courses, for training workshops, as a platform to explore the potential for GPUs to accelerate applications to the petascale and beyond, and as a resource for science and engineering researchers.

For more information on the IACAT cluster, see:
iacat.illinois.edu/resources/cluster/

Moving targets

A research team is utilizing NCSA resources to develop new methods of studying fluid-structure interaction and modeling of turbulence on moving grids.



COUPLED ANALYSIS of fluid-structure interaction (FSI) problems combines fluids, solids, and their interactions in a single-pass simulation with the intent of capturing the true multiphysics behavior of the system. Current computational methods work reasonably well in predicting coupled effects in mildly nonlinear nonlinear FSI problems. However, says Arif Masud, "mathematically non-smooth FSI problems pose great challenge." For general systems where a time accurate simulation is the only authentic approach, high-fidelity computer programs and computer algorithms will be required to take full advantage of the opportunities offered by the developments in hardware, such as the Blue Waters sustained petascale machine to come online in 2011.

Professor Masud and his team in the civil and environmental engineering department at the University of Illinois at Urbana-Champaign are developing mathematically robust and computationally economic FSI techniques with the assistance of NCSA, so researchers can economically obtain accurate solutions. One of their projects tested algorithms modeling aircraft pressure, velocity, and vorticity around YF-17 aircraft. This lightweight fighter jet prototype is the basis for the U.S. Navy's F-18 Hornet and Super Hornet. Using NCSA's Cobalt, the team conducted numerous simulations

Since these computations involved large and dense meshes—the mesh is composed of one million tetrahedral elements with about five million degrees of freedom—Masud turned to NCSA's Advanced Applications Support visualization group to visualize the results. The visualization was especially helpful in method development as it allowed researchers to see the effects of various terms that otherwise could only be indirectly estimated.

"This was an interesting project which required the use of a variety of visualization tools," says visualization programmer Mark Van Moer. "The polygonal aircraft body was extracted from the original mesh using a combination of custom VTK scripts and Blender. The final renderings were done with Kitware's ParaView, a parallel renderer, which is built with Kitware's VTK C++ class library. The data also allowed for a wide variety of vector and scalar visualization techniques."

Masud says the team successfully developed multiscale finite element methods for incompressible Navier-Stokes equations and extended the capability to formulations written in arbitrary Lagrangian-Eulerian frameworks for problems involving moving and deforming spatial domains. The technology was integrated with 2D and 3D adaptive mesh rezoning schemes previously developed. And they have recently extended variational multiscale/stabilized formulation for incompressible Navier-Stokes equations to variational multiscale residual-based turbulence models for large eddy simulation.

This research was funded through the NCSA Faculty Fellows program, which enables campus researchers to collaborate with NCSA.


LOG VORTICITY MAGNITUDE
0.00055
0.0076
0.10
1.40
20
PRESSURE
-0.12
-0.045
0.030
0.10
0.18
AIR PRESSURE ON THE PLANE'S SURFACE
AIR PRESSURE IN SURROUNDING SPACE

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